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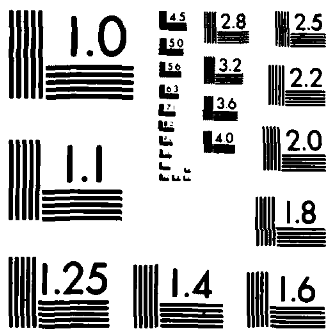

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PERCOLATION AND CRITICAL BEHAVIOUR IN MANY BODY SYSTEMS

FINAL TECHNICAL REPORT

BY

C. DOMB

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ABSTRACT

The most important problem which has been tackled in the past 3 years has been the resolution of the discrepancy between series expansions and renormalization group calculations. Many research workers in different parts of the world have been concerned with this problem. The contribution of the King's College group has been to provide additional terms in the high temperature series expansions for the n-vector model, and to analyse the results taking into account the predictions of the renormalization group. Investigations of the statistical properties of a single polymer chain in 3 dimensions have continued using the Domb-Joyce model. The expansion factor in the two parameter approximation has been calculated for the mean square distance from one end of the chain, the mean square radius of gyration, and the probability of ring closure, as a function of excluded volume. Similar calculations have been undertaken for a two dimensional model. A new investigation has been carried out of the percolation exponent β. Baxter's exact solution for hard hexagons has been used to throw light on the nature of the virial series for hard core fluids.

Fourteen appendices are attached to the original copy of this Technical Report. All are available in the open scientific literature. Copies can also be obtained on request from controlling office.

ABSTRACT

The most important problem which has been tackled in the past 3 years has been the resolution of the discrepency between series expansions and renormalization group calculations. Many research workers in different parts of the world have been concerned with this problem. The contribution of the King's College group has been to provide additional terms in the high temperature series expansions for the n-vector model, and to analyse the results taking into account the predictions of the renormalization group. Investigations of the statistical properties of a single polymer chain in 3 dimensions have continued using the Domb-Joyce model. The expansion factor in the two parameter approximation has been calculated for the mean square distance from one end of the chain, the mean square radius of gyration, and the probability of ring closure, as a function of excluded volume. Similar calculations have been undertaken for a two dimensional model. A new investigation has been carried out of the percolation exponent β. Baxter's exact solution for hard hexagons has been used to throw light on the nature of the virial series for hard core fluids.

A

INTRODUCTION AND SUMMARY

(a) Series Expansions and the Renormalization Group

The introduction of the renormalization group (RG) into critical phenomena by K G Wilson[1] provided an enormous stimulus to progress, and the importance of his work was recognised by the award of a Nobel prize a few months ago. Although the agreement between the initial predictions of the RG and those of series expansions were considered satisfactory at first, further investigations revealed small but persistent discrepancies. For example whereas series expansions predicted $\gamma = 1.250$ for the susceptibility[2], RG estimates were closer[3] to 1.241. This difference would not be too significant if it did not bring into question the whole edifice of hyperscaling relations which is an essential part of the RG treatment. Hence it was of great importance to attempt to resolve the discrepancy.

The Cargese NATO Summer School in July 1980 was devoted to the subject of Phase Transitions, and the above topic was a central feature of discussion at the School. Two members of our group (D S Gaunt and S McKenzie) attended the School and presented papers (Appendices 1 and 2). In view of most of the participants the discussions at the School went a long way towards resolving the discrepancy for the Ising model by providing new terms, and introducing the confluent singularity predicted by the RG. The problem was reviewed by B Nickel[4] at the International Conference on Statistical Mechanics in Edmonton Alberta at the end of August 1980 (STATPHYS 14).

Our own project on the n-vector model was brought to a successful conclusion subsequently, and has achieved the following results for the $n = 3$ (classical Heisenberg model):

3 dimensions	FCC lattice	2 new terms
	SC lattice	2 new terms
	BCC lattice	1 new term

4 dimensions	HFCC lattice	9 terms (all new)
	HSC lattice	3 new terms
	HBCC lattice	11 terms (all new)

The results are analyzed in Appendices 3 and 4.

(b) Polymer Configurations

Some years ago the Principal Investigator initiated a new method of calculating the expansion factor of the mean square end to end length of a polymer chain. The method uses the Domb-Joyce model of a random walk[5] with interactions, and was developed in collaboration with A J Barrett and M Lax. The results were published in a number of papers[6].

The method has now been applied (in collaboration with A J Barrett) to other statistical properties of a polymer chain, the mean square distance from one end, and the probability of ring closure. Virial series were derived for these quantities which were combined with self-avoiding walk data to calculate the expansion factors which were found to be universal (in the terminology of critical phenomena). The results are presented in Appendix 5.

A preliminary step in the calculation of the virial expansion for the radius of gyration was the calculation of mean square distances between points of a random walk when there are restrictions (eg that the walk is a closed loop, or that the end-to-end length is fixed as L). The principal investigator devised a new mathematical method for such calculations based on the use of generating functions (see Appendix 6).

Similar calculations were undertaken in two-dimensions in collaboration with P Ratcliffe. Here an important result established was that the logarithmic terms present in the expansion for the partition function disappear to all orders when a universal quantity like the mean square end-to-end length is

calculated. This is presented in Appendix 7.

A general review of the Domb-Joyce model and the transition from random to self-avoiding walks was given by the principal investigator at a recent Conference on Random Walks held in Washington (see Appendix 8).

(c) Percolation

A number of investigations were initiated in connection with percolation. There is considerable uncertainty about critical exponents. Real space RG estimates have not yet achieved adequate reliability, and the ϵ-expansion which has to start from 6 dimensions can only give qualitative results. A re-examination of the exponent β was undertaken for the site and bond problems using new techniques and extra data. The results are presented in Appendix 9.

A great deal of interest has been focussed recently on the structure of clusters (finite and infinite) in a percolation process. In an effort to throw some light on this problem calculations were undertaken of the mean valence of sites in bond percolation as a function of the concentration (Appendix 10) and of the mean valence of sites in non-percolating clusters in a site percolation process (Appendix 11).

(d) Virial Expansion for Hard-core Fluids

This is an old problem of great difficulty which received new impetus from recent calculations of Kratky[7]. Baram and Luban[8] published an analysis of his results indicating that the first singularity corresponds to the density of closest packing. But Gaunt and Joyce (Appendix 12) and Baxter's exact solution[9] for hard hexagons show how singularities arise in the complex plane which do not make themselves felt until many terms have passed. They suggested that the number of terms available for hard core fluids is too few to draw any reliable conclusions.

(e) General Reviews

One of the most important catalysts to research progress in a fast moving field is the provision of accurate and reliable reviews of progress. The principal investigator undertook the commissioning and editing of such reviews in collaboration with the late M S Green in a series of volumes (1-6) entitled "Phase Transitions and Critical Phenomena". It was generally agreed by workers in the field that these volumes were a great help to them in their work. The last volume on the renormalization group appeared in 1976 and a few years later Mel Green passed away. The principal investigator has now teamed up with a new co-editor, Joel L Lebowitz, to plan a continuation of the series. Two volumes are already in the press (Vol 7 contains reviews of Defect Mediated Phase Transitions, Exactly Solvable Models of Phase Transitions in a Macromolecule, and Dilute Magnetism, and Vol 8 of Critical Behaviour at Surfaces, Finite Size Scaling, and Dynamics of First-order Phase Transitions). The third volume is about to be sent to press and contains reviews on Tricritical Points (experiment and theory) and Field Theory and Statistical Mechanics. In a tribute volume to the late M S Green the principal investigator contributed a historical review of progress in critical phenomena (Appendix 13). He has also prepared a general historical review of percolation processes for a general publication on this topic by the Israel Physical Society (Appendix 14).

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9. R J Baxter J Phys A 13 L61 (1980).

APPENDICES

APPENDIX 1:

High Temperature Series Analysis for the Three-Dimensional Ising Model: A review of some recent work
D S GAUNT

Traditional high temperature series estimates of critical exponents for the three-dimensional Ising model differ from renormalization group theory estimates but by only a small amount. However, the quoted uncertainties in each method are too small to explain the difference in a convincing manner. Reanalysis of the high temperature series has been undertaken by several researchers, whose work we review here, in an attempt to resolve this discrepancy.

APPENDIX 2:

Derivation of High Temperature Series Expansions: Ising Model
SATI MCKENZIE

The derivation of high temperature series expansions for the Ising model, with special reference to the spin 1/2 case is discussed. We shall see how these methods of derivation can be extended to the classical vector model.

APPENDIX 3:

Extended High-Temperature Series for the Classical Heisenberg Model in Three Dimensions
S MCKENZIE, C DOMB AND D L HUNTER

Extended series expansions are derived for the high-temperature susceptibility of the classical Heisenberg model, on three-dimensional lattices. Series coefficients are presented to twelfth order for the simple cubic (SC) and face centred cubic (FCC) lattices and to eleventh order for the body centred cubic (BCC) lattice. Our results are in agreement with earlier calculations apart from a small discrepancy at the tenth order on the FCC lattice. In addition, this work extends earlier series by two terms on the FCC and SC lattices and by one term on the BCC lattice. Extrapolation studies on the extended series are used to obtain revised estimates for the critical points (K_c and the susceptibility exponent (γ)). On the FCC lattice, we also investigate the possibility of a confluent non-analytic correction to the dominant singularity. While the coefficients are consistent with the presence of such a correction term with an exponent (Δ_1) of 0.55, as predicted by renormalisation group (RG) calculations, the amplitude of the correction term appears to be very small compared with that of the first analytic correction term. Our estimate for γ is in excellent agreement with RG predictions, but is somewhat lower than those of Ferer **et al** and Camp and Van Dyke.

APPENDIX 4:

The High-Temperature Susceptibility of the Classical Heisenberg Model in Four Dimensions
S MCKENZIE, C DOMB AND D L HUNTER

The high-temperature susceptibility of the four-dimensional Heisenberg model is studied by the method of series expansions. High-temperature series are presented to order K^9 for the hyper face centred (HFCC) lattice, to order K^{11} for the hyper body centred cubic (HBCC) lattice and to order K^{12} for the hyper simple cubic (HSC) lattice. The last three coefficients for the HSC lattice and all the coefficients for the other two lattices are new. The series are analysed for singularities of the form $t^{-1}|\ln t|^p$, predicted by the renormalisation group theory ($t = 1 - K_c/K$, where K is the high-temperature expansion variable J/kT). Fairly good convergence is obtained for p 0.45 for all three lattices, in agreement with renormalisation group calculations.

APPENDIX 5:

Statistical Properties of a Polymer Chain in the Two-Parameter Approximation
A J BARRETT AND C DOMB

The diagrammatic method developed in a previous paper is used to derive two terms of the virial expansion for the mean square distance from the origin, the mean square radius of gyration, and the probability of ring closure for a lattice model of a simply polymer chain. It is found that the logarithmic terms in the partition function cancel in the virial series for these universal quantities. The universality hypothesis is tested with the numerical data for self-avoiding walks (saw) for different lattices. The virial series is combined with the saw results to provide formulae for the expansion factor as a function of the encluded volume.

APPENDIX 6:

Averages in Restricted Random Walks
C DOMB

In configurational studies of polymer chains one is sometimes concerned with averages in the presence of restrictions, eg that the end-to-end distance of the chain is R. The standard method of calculating such averages is to assume that the separation of all pairs of elements is Gaussian. An alternative method is developed here which uses generating functions and avoids the Gaussian assumption. The results are equivalent asymptotically to those with the Gaussian assumption, but correction terms can be calculated.

APPENDIX 7:

Virial Expansion of a Two-Dimensional Polymer Chain: Cancellation of Logarithmic Terms
C DOMB AND P J RATCLIFFE

A virial expansion is developed for a two-dimensional polymer chain in the two-parameter approximation. Logarithmic terms in the partition function arise from ladder graphs, in contrast to the three-dimensional chain where they are due to non-ladder graphs. It has been possible to show that when the mean square end-to-end distance ($R^2{}_N$) is calculated the logarithmic terms cancel to all orders, thus verifying universality.

APPENDIX 8:

From Random to Self-Avoiding Walks
C DOMB

A brief review will be given of the current situation in the theory of self-avoiding walks (SAW's). The Domb/Joyce model first introduced in 1972 consists of a random walk on a lattice in which each N step configuration has a weighting factor

$$\prod_{i=0}^{N-2} \prod_{j=i+2}^{N} (1 - \omega\delta_{\underline{ij}}) .$$

Here $\underline{i}$ and $\underline{j}$ are the lattice sites occupied by the i-th and j-th points of the walk. When $\omega = 0$ the model reduces to a standard random walk, and when $\omega = 1$ it is a self-avoiding walk. The universality hypothesis of critical phenomena will be used to conjecture the behaviour of the model as a function of ω for large N. The implications for the theory of dilute polymer solutions will be indicated.

APPENDIX 9:

Series Esimate of the Exponent β for Bond Percolation on a Simple Cubic Lattice
D S GAUNT, S G WHITTINGTON AND M F SYKES

The critical exponent β for the bond problem on a simple cubic lattice is analysed by a Pade approximant technique using high-density expansions corresponding to three different definitions of the percolation probability. It is found that $\beta = 0.463 \pm 0.013 - 12\Delta p_c$ where $\Delta p_c = p_c - 0.247$. The need for more precise estimates of the criticial density p_c is emphasised.

APPENDIX 10:

Valences of Sites in Percolating and Non-percolating Clusters
S G WHITTINGTON, K M MIDDLEMISS, G M TORRIE AND D S GAUNT

We present some exact enumeration data and approximate Pade mimic functions for the p dependence of the fraction of sites in finite clusters for thesquare lattice site problem having given valence. In addition, we report Monte-Carlo results on the corresponding quantities for sites in infinite clusters and use these data to investigate the degree of ramification of infinite clusters at and above the percolation threshold.

APPENDIX 11:

Valences of Sites in Bond Percolation
S G WHITTINGTON, K M MIDDLEMISS AND D S GAUNT

We present calculations for the fraction of sites with given valence in finite and infinite clusters in the Bethe approximation, for a lattice of coordination number Q, and compare these results with series analysis results for the bond percolation problems on the square and simple cubic lattices.

APPENDIX 12:

Virial Expansions for Hard-Core Fluids
D S GAUNT AND G S JOYCE

We discuss some of the difficulties involved in drawing conclusions about the asymptotic behaviour of the virial coefficients for a hard-core fluid when only the first few coefficients are known. Particular consideration is given to the recent work of Baram and Luban for hard discs and spheres, and that of Baxter for hard hexagons on the triangular lattice.

APPENDIX 13:

Critical Phenomena - A Model Illustration of Scientific Method
C DOMB

A historical survey is undertaken of the development of critical phenomena from the early days of Andrews and van der Waals to the modern era of the renormalization group. The history is divided into 4 periods; the classical pre-Onsager period (1869-1944); the Onsager revolution (1944-1965); the reconciliation of Onsager with van der Waals (1965-1971); and the renormalization group (1971-). Special attnetion is paid to the relation between experiment and theory, the new concepts required to explain new phenomena, the empirical development of a theoretical framework which adequately described the experimental results, and the final theoretical developments which enabled them to be understood.

APPENDIX 14:

The Percolation Phase Transition

C DOMB

This article aims to provide an introduction to the concepts of percolation for the non-specialist, who should then be in a position to understand the more specialised articles in the volume. A brief survey if first given of the development of percolation theory during the past 25 years. The following topics are discussed: bond and sire processes, perimeter polynomials, analogy with the Ising model, pair connectedness, series expansion methods, Monte Carlo methods, exploration of critical behaviour, scaling in the critical region, lattice animals, percolation clusters, renormalization group, correlated percolation, continuum percolation, fractal dimensions and self similarlity.

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